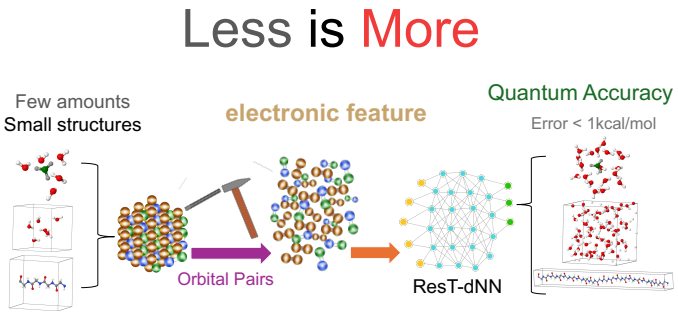
Deep Learning Electron Correlation of Molecules and Solids

Wai-Pan Ng,[1] Zili Zhang,[1] Qiujiang Liang[1,2] and Jun Yang* [1,2,3,4]

[1] *Department of Chemistry, The University of Hong Kong, Hong Kong, China;*
[2]*Hong Kong Quanutm AI Lab Limited, Hong Kong, China;*
[3]*State Key Laboratory of Synthetic Chemistry, The University of Hong Kong, Hong Kong, China;*
[4]*HKU-CAS Joint Laboratory on New Materials, The University of Hong Kong, Hong Kong, China*

juny@hku.hk

Accurate quantum chemistry prediction of electron correlation energies is prohibitively expensive for macromolecules when explicitly solving post-Hartree-Fock equations. Existing machine learning models attempt to predict the energies of large molecules by training small molecules, but eventually fail to retain high accuracy as the errors increase with system size. We have developed a sparse quantum-feature-informed deep neural network model [1, 2] that removes both feature and data redundancies on only hundred-scale data of small molecules, and we target correlation energies at chemical accuracy on par with direct MP2 and CCSD computations across varying molecular compositions, bond types, geometries and lattice phases. Our neural network model is thus data efficient and transferable for a variety of molecules and periodic solids, including short alkanes, long glycine chains, dimeric organic and biologic molecules, water clusters of different sizes and shapes, and ice solid in different phases. The results suggest that an extremely compact correlation feature set [3], which is clearly very poor for any direct post-Hartree-Fock calculations, has a prominent advantage in reserving important electron correlation patterns and it is possible to make chemically accurate transferable predictions. We further applied our neural network model to score and rank the protein-ligand interactions that are critical and still remain one of the greatest challenges for drug discovery. Our work represents an important step forward in the quest for cost-effective, highly accurate and transferable neural network models in quantum chemistry, bridging the electronic structure patterns between small and large systems.



Scheme: Trnasferable Neural Network Model for Ab Initio Quantum Chemistry

References

1. Ng, W.-P.; Zhang, Z.; Yang, J. *J. Chem. Theory Comput.* **2025 (ASAP)**, doi: 10.1021/acs.jctc.4c01261.
2. Ng, W.-P.; Liang, Q.; Yang, J. *J. Chem. Theory Comput.* **2023**, *19*, 5439 – 5449.
3. Liang, Q.; Yang, J. *J. Chem. Theory Comput.* **2021**, *17*, 6841 – 6860.